

# Generalized detailed Fluctuation Theorem under Nonequilibrium Feedback control

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It has been shown recently that the Jarzynski equality is generalized under nonequilibrium feedback control [T. Sagawa and M. Ueda, *Phys. Rev. Lett.* **104**, 090602 (2010)]. The presence of feedback control in physical systems should modify both Jarzynski equality and detailed fluctuation theorem [K. H. Kim and H. Qian, *Phys. Rev. E* **75**, 022102 (2007)]. However, the generalized Jarzynski equality under forward feedback control has been proved by consider that the physical systems under feedback control should locally satisfies the detailed fluctuation theorem. We use the same formalism and derive the generalized detailed fluctuation theorem under nonequilibrium feedback control. It is well known that the exponential average in one direction limits the calculation of precise free energy differences. The knowledge of measurements from both directions usually gives improved results. In this aspect, the generalized detailed fluctuation theorem can be very useful in free energy calculations for system driven under nonequilibrium feedback control.

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Recent development in statistical physics relationships describe nonequilibrium dynamics in terms of equalities [1–3]. In particular, the Jarzynski's equality [1] and the Crooks detailed fluctuation theorem [2] can be used to calculate equilibrium free energy differences from nonequilibrium work distribution. A system initially at equilibrium with temperature (inverse)  $\beta = 1/k_B T$  ( $k_B$  is the Boltzmann constant) is externally driven from its initial state to final state by nonequilibrium process satisfies the detailed fluctuation theorem  $P(W)/P(-W) = \exp(\beta(W - \Delta F))$  and its integrated version, the Jarzynski equality  $\langle \exp(-\beta W) \rangle = \exp(-\beta \Delta F)$ . Where  $W$  denotes the work performed on the system,  $\Delta F$  is the free energy difference of the system between its final and initial equilibrium states and  $P(\pm W)$  is the work probability distribution in forward (+) and reverse (-) direction. The (exponential) average  $\langle \cdot \rangle$  is taken over the ensemble of nonequilibrium trajectories. These relationships has been verified in experiments [4, 5] as well as simulations [6, 7] and widely used in many branches of Science (see, eg.[8]).

Various experiments and simulations has been performed by adopting a suitable time-dependent driving scheme described by an external control switching protocol. Even though the Jarzynski equality and the detailed fluctuation theorem are valid for any time-dependent driving scheme, the efficiency of a nonequilibrium switching simulations which use these relationships to estimate precise free energy difference is depends on the switching function [9]. The practical difficulties faced in precise calculation of free energy differences in simulations [10] initiated further developments in these theories [11]. In

our recent work, we have discussed the analogy between the optimized switching free energy simulation and the nonequilibrium systems which are subjected to a feedback control [12].

The evolution of the physical systems can be modified or controlled by repeated operation of an external agent called controller [13, 14]. In contrast to open loop controller which operates on the system blindly, the feedback or closed loop controllers use information about the state of the system. The feedback is the process performed by the controller of measuring the system, deciding on the action given the measurement output, and acting on the system [15]. For example, in a single molecule Atomic Force Microscopy experiment, the external agent is an electric feedback circuit which detects the motion of the cantilever and manipulate the control force proportional to its velocity [16]. The proper utilization of the information about the state of the system in feedback control effectively improves the system performance [13–17]. However, the presence of feedback control in physical system modifies both the Jarzynski equality and the fluctuation theorem [16].

Recently, the Jarzynski equality is generalized to an experimental condition in which the system is driven between two equilibrium state via nonequilibrium process under forward feedback control [18]. Since the work that performed on a thermodynamic system can be lowered by feedback control [18], this feedback mechanism can be helpful in simulation for sampling rare trajectories and calculate precise free energy differences [12]. The equilibrium free energy difference for the driven system (which locally satisfies the detailed fluctuation theorem) under nonequilibrium feedback control in forward direction can be calculated from the generalized Jarzynski equality [18]

$$\langle e^{-\sigma - I} \rangle = 1, \quad (1)$$

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where  $\sigma = \beta(W - \Delta F)$  and  $I$  is the mutual information measure obtained by the feedback controller [18]. The average is taken from the work distribution in forward direction with feedback control.

The second law of thermodynamics can be quantitatively described by the fluctuation theorem which are closely related to the Jarzynski equality. If the experiments or simulations has been performed under feedback control, both the Jarzynski equality and the fluctuation theorem should be extended [16]. However, the generalized Jarzynski equality (Eq.1) under forward feedback control has been proved by consider that the physical systems under feedback control should locally satisfies the detailed fluctuation theorem [18]. In this letter, we use the same formalism and derive the generalized detailed fluctuation theorem under nonequilibrium feedback control. In order to calculate the free energy differences precisely in simulations one require information of work distribution in both forward and reverse direction [19–21]. In this aspect, one needs the generalized detailed fluctuation theorem under nonequilibrium feedback control.

The feedback control enhances our controllability of small thermodynamics systems [13–17]. At a given time, the controller measure the partial state of the system. The result of the measurement determines the action the control will take. The additional information on the system provided by the measurement further determines the system states. Suppose, the controller perform a measurements on a stochastic thermodynamics system at time  $t_m$ . Let  $\Gamma_m$  be the phase-space point of the system at that time,  $P[\Gamma_m]$  its probability and  $y$  the measurement. Depends on the controller measurements the measurement outcome  $y$  occurs with probability  $P[y]$  [18]. The information obtained by the controller measurement can be characterized by the mutual (feedback) information measure [18, 22],

$$I[y, \Gamma_m] = \ln \left[ \frac{P[y|\Gamma_m]}{P[y]} \right], \quad (2)$$

where  $P[y|\Gamma_m]$  is the conditional probability of obtaining outcome  $y$  on condition that the state of the system is  $\Gamma_m$ . The above equation is rewritten as,

$$e^{I[y, \Gamma_m]} = \frac{P[y|\Gamma_m]}{P[y]}. \quad (3)$$

In experiments and simulations, the free energy difference between the two equilibrium states can be calculated in general by pulling the sytem from one equilibrium state to another state along a switching path. The path connecting the two states in the time period  $\tau$  will be parameterized using the variable  $\lambda$ , with  $0 \leq \lambda \leq 1$ . The switching rate describes the nature of the switching process to be an equilibrium (infinitely slow) or nonequilibrium (fast). If the experiments performed under feedback control, the switching control parameter  $\lambda$  depends

on the outcome  $y$  after  $t_m$  [18]. That is, whenever the controller made measurements, there is a corresponding changes in the switching parameter for next time step, which is denoted as  $\lambda_{(t;y)}$ . Between the every stages of the controller measurements, the value of outcome  $y$  is fixed and the corresponding switching parameter  $\lambda_{(t;y)}$  doesnot change. In this time interval for each stages of  $\lambda_{(t;y)}$ , we consider the system should locally satisfies the detailed fluctuation theorem [18],

$$\frac{P_{\lambda_{(t;y)}}[\Gamma(t)]}{P_{\lambda_{(t;y)}^\dagger}[\Gamma^\dagger(t)]} = e^{\sigma[\Gamma(t)]}, \quad (4)$$

where  $P_{\lambda_{(t;y)}}[\Gamma(t)]$  is the probability of obtaining the outcome  $y$  in forward direction with switching protocol  $\lambda_{(t;y)}$  and  $P_{\lambda_{(t;y)}^\dagger}[\Gamma^\dagger(t)]$  is the probability of obtaining the same outcome  $y$  [18] in reversed direction of phase point,  $\Gamma^\dagger(t)$ , with corresponding switching protocol  $\lambda_{(t;y)}^\dagger$ . Here,  $\sigma[\Gamma(t)]$  is the work value obtained in the forward direction and its time reversal work value

$$\sigma[\Gamma^\dagger(t)] = -\sigma[\Gamma(t)]. \quad (5)$$

Let  $P_F[\tilde{X}] \equiv P_F[\sigma[\tilde{\Gamma}], I[\tilde{y}, \tilde{\Gamma}]]$  be the the joint probability of obtaining the work value  $\sigma[\tilde{\Gamma}]$  for a given feedback information measure  $I[\tilde{y}, \tilde{\Gamma}]$  of measurement outcome  $\tilde{y}$  in forward direction. Due to the repeated measurements of the controller, the particular measurement outcome  $\tilde{y}$  may occurs in various stages of the experiment. In analogous to previous studies [23, 24], this (joint) probability can be obtained from the nonequilibrium ensemble of variable (forward) switching trajectories as,

$$P_F[\tilde{X}] = \int P[y'|\Gamma'_m] P_{\lambda_{(t;y')}}[\Gamma(t)] \delta(I[y', \Gamma'_m] - I[\tilde{y}, \tilde{\Gamma}]) \delta(\sigma[\Gamma(t)] - \sigma[\tilde{\Gamma}]) dy' D[\Gamma(t)], \quad (6)$$

where  $\delta(x)$  is the Dirac delta function which has a property  $\delta(-x) = \delta(x)$ . It should be noted that  $y'$  and  $\Gamma'_m$  in the conditional probabilities are dummy variables and it has appropriate values for each outcome of the controller measurements, see Eq.(3).

Combining Eq.(3) and Eq.(4), then Eq.(6) becomes,

$$\begin{aligned} P_F[\tilde{X}] &= \int e^{\sigma[\Gamma(t)] + I[y', \Gamma'_m]} P[y'] P_{\lambda_{(t;y')}^\dagger}[\Gamma^\dagger(t)] \\ &\quad \delta(I[y', \Gamma'_m] - I[\tilde{y}, \tilde{\Gamma}]) \delta(\sigma[\Gamma(t)] - \sigma[\tilde{\Gamma}]) \\ &\quad dy' D[\Gamma(t)], \\ P_F[\tilde{X}] &= e^{\sigma[\tilde{\Gamma}] + I[\tilde{y}, \tilde{\Gamma}]} \int P[y'] P_{\lambda_{(t;y')}}[\Gamma^\dagger(t)] \\ &\quad \delta(I[y', \Gamma'_m] - I[\tilde{y}, \tilde{\Gamma}]) \delta(\sigma[\Gamma(t)] - \sigma[\tilde{\Gamma}]) \\ &\quad dy' D[\Gamma(t)]. \end{aligned} \quad (7)$$

Let  $P_R[\tilde{X}^\dagger] \equiv P_R[-\sigma[\tilde{\Gamma}], I[\tilde{y}^\dagger, \tilde{\Gamma}]]$  be the the joint probability of obtaining the work value  $-\sigma[\tilde{\Gamma}]$  for a given feedback information measure  $I[\tilde{y}^\dagger, \tilde{\Gamma}]$  of measurement outcome  $\tilde{y}^\dagger$  in reverse direction. This (joint) probability can be obtained from the nonequilibrium ensemble of variable (reverse) switching trajectories as,

$$P_R[\tilde{X}^\dagger] = \int P[y'|\Gamma'_m] P_{\lambda_{(t;y')}}^\dagger[\Gamma^\dagger(t)] \delta(I[y', \Gamma'_m] - I[\tilde{y}^\dagger, \tilde{\Gamma}]) \delta(\sigma[\Gamma^\dagger(t)] + \sigma[\tilde{\Gamma}]) dy' D[\Gamma^\dagger(t)]. \quad (8)$$

To this end we will use above equations and derive the generalized detailed fluctuation theorem under feedback control either in forward direction [18] or both directions as follows.

If the system has same feedback control in both directions then under the controller measurements condition  $I[\tilde{y}^\dagger, \tilde{\Gamma}] = I[\tilde{y}, \tilde{\Gamma}]$  and using Eq.(3), we can rewrite Eq.(8) as,

$$P_R[\tilde{X}^\dagger] = e^{I[\tilde{y}, \tilde{\Gamma}]} \int P[y'] P_{\lambda_{(t;y')}}^\dagger[\Gamma^\dagger(t)] \delta(I[y', \Gamma'_m] - I[\tilde{y}, \tilde{\Gamma}]) \delta(\sigma[\Gamma^\dagger(t)] + \sigma[\tilde{\Gamma}]) dy' D[\Gamma^\dagger(t)]. \quad (9)$$

Since  $\delta(-x) = \delta(x)$  and  $D[\Gamma^\dagger(t)] = D[\Gamma(t)]$  [18], combining Eq.(5) and Eq.(9) in Eq.(7) we can obtain the generalized detailed fluctuation theorem under feedback control in both direction as

$$P_F[\tilde{X}] = e^{\sigma[\tilde{\Gamma}] + I[\tilde{y}, \tilde{\Gamma}]} P_R[\tilde{X}^\dagger] e^{-I[\tilde{y}, \tilde{\Gamma}]}, \quad \frac{P_F[\tilde{X}]}{P_R[\tilde{X}^\dagger]} = e^{\sigma[\tilde{\Gamma}]}. \quad (10)$$

The above equation can be written simply as

$$\frac{P_F[\sigma, I]}{P_R[-\sigma, I]} = e^\sigma. \quad (11)$$

Our result shows that for a given feedback information measure  $I$  in both directions, the physical system under feedback control satisfies the detailed fluctuation theorem  $\frac{P_F[\sigma]}{P_R[-\sigma]} = e^\sigma$ . Since the feedback control enhances our controllability of small thermodynamics systems, the proper choice of feedback mechanism in free energy simulations can be useful for precise free energy estimates instead looking for optimized switching protocols [12].

If the system has feedback control only in forward direction, the generalized detailed fluctuation theorem under forward feedback control can be obtained from the following reverse experimental condition. Based on the informations about switching protocols for each outcome in forward feedback control experiment, without feedback

control, we can perform same variable switching protocols experiment in reverse direction [18]. This is equivalent as an open loop controller which operates on the system in reverse direction. In such a case,  $P[y'|\Gamma'_m] = P[y']$  in reverse direction and the open loop controller implicitly has information about the forward feedback information measure  $I[\tilde{y}, \tilde{\Gamma}]$  for corresponding switching parameter,  $\lambda_{(t;y')}^\dagger$ , in reverse direction, see Eqs.(3) and (4). Then, we can write Eq.(8) as

$$P_R[\tilde{X}^\dagger] = \int P[y'] P_{\lambda_{(t;y')}}^\dagger[\Gamma^\dagger(t)] \delta(I[y', \Gamma'_m] - I[\tilde{y}, \tilde{\Gamma}]) \delta(\sigma[\Gamma^\dagger(t)] + \sigma[\tilde{\Gamma}]) dy' D[\Gamma^\dagger(t)]. \quad (12)$$

As similar to earlier derivation, combining Eq.(5) and Eq.(12) in Eq.(7) we can obtain the generalized detailed fluctuation theorem under forward feedback control as

$$P_F[\tilde{X}] = e^{\sigma[\tilde{\Gamma}] + I[\tilde{y}, \tilde{\Gamma}]} P_R[\tilde{X}^\dagger], \quad \frac{P_F[\tilde{X}]}{P_R[\tilde{X}^\dagger]} = e^{\sigma[\tilde{\Gamma}] + I[\tilde{y}, \tilde{\Gamma}]}. \quad (13)$$

In order to prove the generalized Jarzynski equality under forward feedback control, we measure the quantity,

$$\langle e^{-\sigma-I} \rangle = \int P_F[\tilde{X}] e^{-\sigma[\tilde{\Gamma}] - I[\tilde{y}, \tilde{\Gamma}]} d\tilde{y} d\tilde{\Gamma}.$$

From Eq.(13),

$$\langle e^{-\sigma-I} \rangle = \int P_R[\tilde{X}^\dagger] d\tilde{y} d\tilde{\Gamma} = 1, \quad (14)$$

we obtained the generalized Jarzynski equality under forward feedback control [18]. In order to get more insight of forward mutual information measure, we calculate the quantity [18]

$$\langle e^{-\sigma} \rangle = \int P_F[\tilde{X}] e^{-\sigma[\tilde{\Gamma}]} d\tilde{y} d\tilde{\Gamma}$$

Using Eq.(13), the average of above equation can be written as

$$\begin{aligned} \langle e^{-\sigma} \rangle &= \int P_R[\tilde{X}^\dagger] e^{I[\tilde{y}, \tilde{\Gamma}]} d\tilde{y} d\tilde{\Gamma} \\ &= \int P_R[\tilde{X}^{\star\dagger}] d\tilde{y} d\tilde{\Gamma}, \\ &= \gamma, \end{aligned} \quad (15)$$

where  $\gamma = \int P_R[\tilde{X}^{\star\dagger}] d\tilde{y} d\tilde{\Gamma}$  is the feedback control characteristics which is a measure of the correlation between the dissipation and the information [18] and  $P_R[\tilde{X}^{\star\dagger}] =$

$P_R[\tilde{X}^\dagger]e^{I[\tilde{y}, \tilde{\Gamma}]}$  is the special case [18] of the joint probability distribution in reverse direction.

Even though there is no feedback control in reverse direction, due to the implementation of variable (reverse) switching protocols in accordance with forward feedback control experiment, the forward mutual information measure can also be obtained from the reverse direction as

$$I[\tilde{y}, \tilde{\Gamma}] = \ln \left[ \frac{P_R[\tilde{X}^{\star\dagger}]}{P_R[\tilde{X}^\dagger]} \right]. \quad (16)$$

In conclusion, we have derived the generalized detailed fluctuation theorem under nonequilibrium feedback control. It is well known that the exponential average in one direction limits the accurate calculation of free energy differences in simulation. The knowledge of measurements from both directions usually gives improved results. Thus, the generalized detailed fluctuation theorem can be very useful in free energy simulation for system driven under nonequilibrium feedback control.

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- [1] C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997).
  - [2] G. E. Crooks, Phys. Rev. E **60**, 2721 (1999); Phys. Rev. E **61**, 2361 (2000).
  - [3] D. J. Evans, E. G. D. Cohen and G. P. Morriss, Phys. Rev. Lett. **71**, 2401 (1993); G. Gallavotti and E. G. D. Cohen, Phys. Rev. Lett. **74**, 2694 (1995); C. Maes, J. Stat. Phys. **95**, 367 (1999); C. Jarzynski, J. Stat. Phys. **98**, 77 (2000); T. Hatano and S. -I. Sasa, Phys. Rev. Lett. **86**, 3463 (2001); T. Harada and S. -I. Sasa, Phys. Rev. Lett. **95**, 130602 (2005); M. Esposito and C. Van den Broeck, Phys. Rev. Lett. **104**, 090601 (2010).
  - [4] J. Liphardt, S. Dunmont, S. B. Smith, I. Jr. Tinoco and C. Bustamante, Science **296**, 1832 (2002).
  - [5] D. Collin, F. Ritort, C. Jarzynski, S. B. Smith, I. Jr. Tinoco and C. Bustamante, Nature **437**, 231 (2005).
  - [6] S. Park, F. K. Araghi, E. Tajkhorshid and K. Schulten, J. Chem. Phys. **119**, 3559 (2003).
  - [7] I. Kosztin, B. Barz and L. Janosi, J. Chem. Phys. **124**, 064106 (2006).
  - [8] S. Vemparala, L. Saiz, R. G. Eckenhoff and M. L. Klein, Biophys. J. **91**, 2815 (2006).
  - [9] M. de Koning, J. Chem. Phys. **122**, 104106 (2005); T. Schmiedl and U. Seifert, Phys. Rev. Lett. **98**, 108301 (2007). A. G. Marin, T. Schmiedl and U. Seifert, J. Chem. Phys. **129**, 024114 (2008); H. Then and A. Engel, Phys. Rev. E **77**, 041105 (2008); P. Geiger and C. Dellago, Phys. Rev. E **81**, 021127 (2010).
  - [10] F. M. Ytreberg and D. M. Zuckerman, J. Comput. Chem. **25**, 1749 (2004); D. D. L. Minh, Phys. Rev. E **74**, 061120 (2006); G. E. Lindberg, T. C. Berkelbach and F. Wang, J. Chem. Phys. **130**, 174705 (2009).
  - [11] S. Vaikuntanathan and C. Jarzynski, Phys. Rev. Lett. **100**, 190601 (2008).
  - [12] M. Ponmurugan, arXiv:Cond-mat/1005.3104.
  - [13] F. J. Cao, L. Dinis and J. M. R. Parrondo, Phys. Rev. Lett. **93**, 040603 (2004); B. J. Lopez, N.J. Kuwada, E. M. Craig, B. R. Long and H. Linke, Phys. Rev. Lett. **101**, 220601 (2008); M. Bonaldi et al., Phys. Rev. Lett. **103**, 010601 (2009). K. Maruyama, F. Nori and V. Vedral, Rev. Mod. Phys. **81**, 1 (2009); T. Sagawa and M. Ueda, Phys. Rev. Lett. **102**, 250602 (2009).
  - [14] J. Bachhoefer, Rev. Mod. Phys. **77**, 783 (2005).
  - [15] F. J. Cao and M. Feito, Phys. Rev. E **79**, 041118 (2009);
  - [16] K. H. Kim and H. Qian, Phys. Rev. Lett. **93**, 120602 (2004); K. H. Kim and H. Qian, Phys. Rev. E **75**, 022102 (2007);
  - [17] T. Sagawa and M. Ueda, Phys. Rev. Lett. **100**, 080403 (2008).
  - [18] T. Sagawa and M. Ueda, Phys. Rev. Lett. **104**, 090602 (2010).
  - [19] M. R. Shirts, E. Bair, G. Hooker and V. S. Pande, Phys. Rev. Lett. **91**, 140601 (2003).
  - [20] M. R. Shirts and V. S. Pande, J. Chem. Phys. **122**, 144107 (2005).
  - [21] F. M. Ytreberg, R. H. Swendsen and D. M. Zuckerman, J. Chem. Phys. **125**, 184114 (2006).
  - [22] C. Beck, Contemporary Phys. **50**, 495 (2009).
  - [23] C. Jarzynski and D. K. Wojcik, Phys. Rev. Lett. **92**, 230602 (2004).
  - [24] A. B. Adib, *Exact Results in Nonequilibrium statistical Mechanics: Formalism and Application in Chemical Kinetics and Single-Molecule Free Energy Estimation*, Ph.D thesis, Brown University, Providence (2006).